Isogermafurenolide

Inchi: InChI=1S/C15H20O2/c1-6-15(5)8-13-11(7-12(15)9(2)3)10(4)14(16)17-13/h6,12-13H,1-2,
InchiKey: IEOHWPUTLCTSCQ-JHIQODARSA-N
Formula: C15H20O2
SMILES: C=CC1(C)CC2OC(=O)C(C)=C2CC1C(=C)C
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	116.54	kJ/mol	Joback Method
hf	-224.70	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	56.98	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.407		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1869.00		NIST Webbook
tb	661.59	K	Joback Method
tc	894.35	K	Joback Method
tf	406.90	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.58	J/mol×K	661.59	Joback Method
cpg	568.19	J/mol×K	700.38	Joback Method
cpg	586.77	J/mol×K	739.18	Joback Method
cpg	604.46	J/mol×K	777.97	Joback Method
cpg	621.42	J/mol×K	816.76	Joback Method
cpg	637.79	J/mol×K	855.56	Joback Method
cpg	653.71	J/mol×K	894.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R424185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume